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Bloch oscillations of a soliton in a molecular chain

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Abstract. The paper presents results of numerical experiments simulating Bloch oscillations of solitons in a deformable molecular chain in a constant electric field. By the example of a homogeneous polynucleotide chain it is shown that the system under consideration can demonstrate complicated dynamical regimes when at the field intensities less than a certain critical value, a soliton as a whole exhibits oscillations, while at the field intensities exceeding the threshold, a soliton turns to a breather which oscillates. It is shown that the motion of a charge in a deformable chain is infinite as contrasted to that in a rigid chain.

PACS. 71.20.Rv Polymers and organic compounds – 72.80.Le Polymers; organic compounds (including organic semiconductors)

It is well known that an electron occurring in an ideal rigid periodic molecular chain or in a solid state superlattice exhibits Bloch oscillations in response to a constant electric field [1]-[5]. In an external time-periodic field, motion of a charge along a rigid chain can be both infinite and finite (dynamical localization) [6]-[10]. In a deformable crystal chain the role of an external field is played by oscillations of the lattice nodes which can be presented as superposition of plane travelling waves, or phonons. In this case the motion of an electron along the chain is thought to be infinite since the electron scatters on phonons and Bloch oscillations do not take place [11].

It is common knowledge that in quasi-one-dimensional molecular chains interaction of an electron with lattice oscillations is not weak. Therefore we cannot safely assume that the electron wave function goes off phase (in view of scattering of the electron on phonons) and Bloch oscillations fail.

To clear up this point we consider the case when a charge placed in a molecular chain transits to a soliton state as a result of interaction with lattice oscillations. This occurs, for example, in homogeneous polynucleotide chains where the charge motion is described by Holstein Hamiltonian in which each site presents a nucleotide pair considered as a harmonical oscillator [12]-[14]:

$$\begin{aligned} &\hat{H} = \hat{H}_h + \hat{T}_k + \hat{U}_p\,, \\ &\hat{H}_h = \nu\sum_{n=1}^{N}(a_n^+ a_{n-1} + a_n^+ a_{n+1}) + \sum_{n=1}^{N}\alpha_n a_n^+ a_n\,, \\ &\hat{T}_k = \sum_{n=1}^{N}\frac{\hat{P}_n^2}{2M},\ \ \hat{U}_p = \sum_{n=1}^{N}k\frac{q_n^2}{2},\ \ \alpha_n = \alpha' q_n + n\hbar\omega_B. \end{aligned} \qquad (1)$$

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Here $\hat{H}_h$ - is a Hamiltonian of a charged particle, a_n^+, a_n - are operators of creation and annihilation of the charge on site n, ν - is the matrix element of the transition from the n - th site to the $n \pm 1$ - site, α_n - is the energy of the particle at the n - th site, $\hbar\omega_B = e\mathcal{E}a$, where $\mathcal{E}$ - is the intensity of the electric field, e - is the electron charge, a - is the distance between neighboring bases. $\hat{T}_k$ - is an operator of the kinetic energy of sites, $\hat{U}_p$ - is the potential energy of sites, $\hat{P}_n$ - is an impulse operator canonically conjugated to the displacement q_n, M - is the effective mass of the site, k - is an elastic constant, α' - is the particle-site displacement coupling constant.

We can pass on to semi classical description of the wave function of the system $|\Psi(t)\rangle$ as an expansion over coherent states:

$$|\Psi(t)\rangle = \sum_{n=1}^{N} b_n(t) a_n^+ \exp\Big\{-\frac{i}{\hbar}\sum_j\Big[\beta_j(t)\hat{P}_j - \pi_j(t)q_j\Big]\Big\}|0\rangle, \quad (2)$$

where $|0\rangle$ - is the vacuum wave function and the quantities $\beta_j(t)$ and $\pi_j(t)$ satisfy the relations:

$$\langle\Psi(t)|q_n|\Psi(t)\rangle = \beta_n(t), \quad \langle\Psi(t)|\hat{P}_n|\Psi(t)\rangle = \pi_n(t). \quad (3)$$

Dynamical equations for the quantities $b_n(t)$ and $\beta_n(t)$ resulting from (1) - (3) have the form :

$$i\hbar\dot{b}_n = \alpha_n b_n + \nu(b_{n-1} + b_{n+1}), \quad (4)$$

$$M\ddot{\beta}_n = -\gamma\dot{\beta}_n - k\beta_n - \alpha'|b_n|^2. \quad (5)$$

Equations (4) are Schrödinger equations where b_n is the amplitude of the particle localization at the n - th site. Equations (5) are classical motion equations describing dynamics of nucleotide pairs with regard for dissipation,

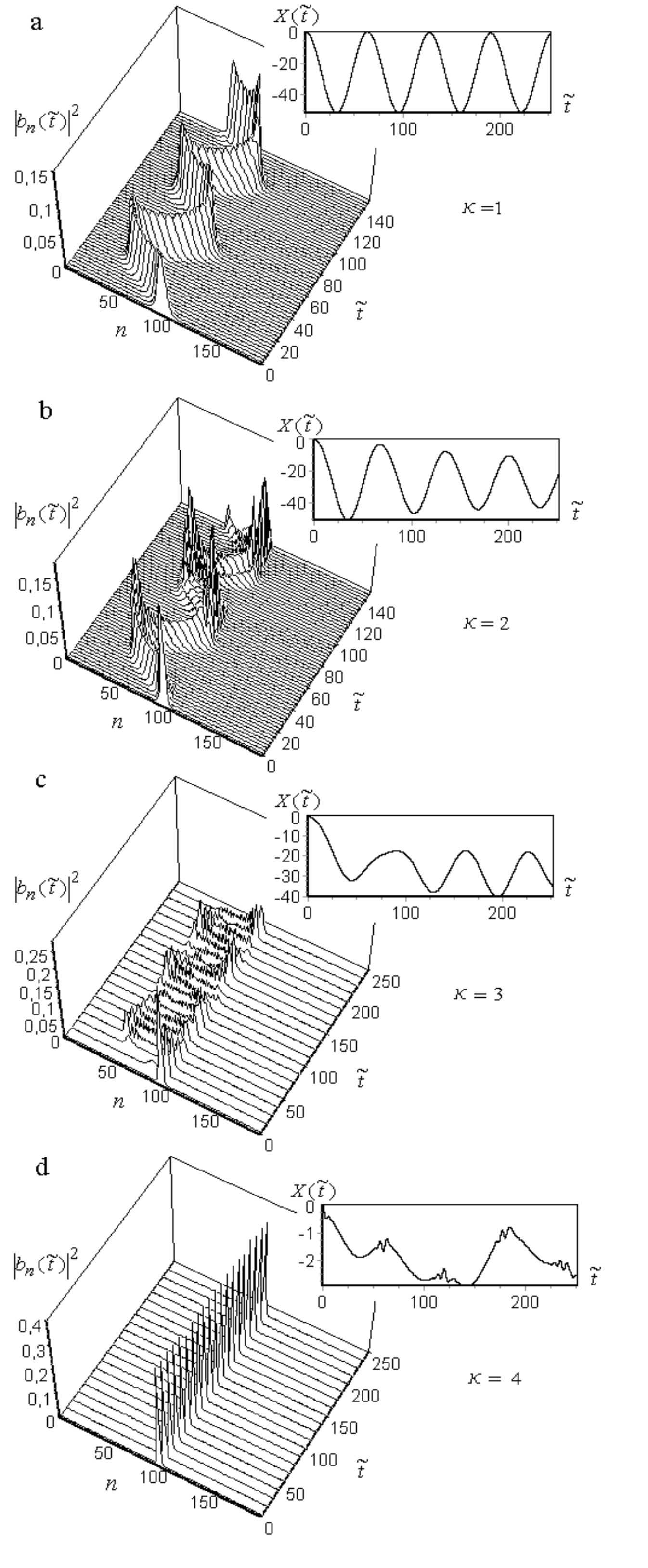

Fig. 1. Oscillatory motions of a soliton for some values of parameter $\kappa(\kappa=1,2,3,4)$ at the electric field intensity $E=0.1$. The length of the homogeneous nucleotide chain is $N=201$, $\widetilde{t}=t/\tau$, $\tau=10^{-14}sec$, $\widetilde{\omega}'=0.006$, $\widetilde{\omega}=0.01$, $\eta=1.276$. ($\widetilde{\omega}'=\omega'\tau$, $\omega'=\gamma/M=6\cdot 10^{11}sec^{-1}$ [12], $\widetilde{\omega}=\omega\tau$).

where γ is friction coefficient. We believe that a semiclassical description in which motion of a charge along a chain is described by quantum motion equations (4) and motion of individual nucleotides is presented by classical motion equations (5) is valid in view of a large nucleotide mass ($\approx$ 300 proton mass).

In the case of a rigid chain, when $\alpha'=0$ the solution of the system (4), (5) will be [15], [16]:

$$b_n(t)=\sum_{m=-\infty}^{\infty} b_m(0)(-i)^{n-m}e^{-i(n+m)\omega_B t/2}J_{n-m}\left(\xi(t)\right),$$
$$\xi(t)=\frac{4\nu}{\hbar\omega_B}\sin\left(\frac{\omega_B t}{2}\right), \qquad (6)$$

$J_n(x)$ - is Bessel function of the first kind. Solution (6) corresponds to Bloch oscillations of a particle in the chain affected by an electric field for which the particle's centre mass:

$$X(t)=\sum_{n=1}^{N}|b_n(t)|^2 na, \qquad (7)$$

demonstrates periodic oscillations at the frequency of ω_B:

$$X(t)=X(0)+\frac{2a\nu}{\hbar\omega_B}|S_0|\left(\cos\theta_0-\cos(\omega_B t+\theta_0)\right),$$
$$S_0=\sum_{m=-\infty}^{\infty} b_m^*(0)b_{m-1}(0)=|S_0|\,e^{i\theta_0}, \qquad (8)$$
$$X(0)=a\sum_{m=-\infty}^{\infty} m|b_m(0)|^2,$$

where a is the distance between neighboring nucleotides, which for DNA is equal to $3.4\mathring{A}$.

For $\alpha'\neq 0$ in the absence of an electric field, a stationary solution of equations (4), (5) corresponds to a localized state of a soliton type. To study the evolution of a soliton state in an electric field we will use an initial charge density distribution such that:

$$|b_n(0)|=\frac{\sqrt{2}}{4}\cosh^{-1}\left(\frac{\kappa(n-n_0)}{4\eta}\right), \qquad (9)$$
$$n_0=\frac{N}{2}+1, \quad \eta=\frac{\nu\tau}{\hbar}, \quad \kappa=\frac{\tau\alpha'^2}{k\hbar}.$$

Initial values of x^0 and y^0 ($b_n=x_n+iy_n$) for $\nu>0$ have the form:

$$x_n^0=|b_n(0)|(-1)^n\Big/\sqrt{2}\,,\;\; y_n^0=|b_n(0)|(-1)^{n+1}\Big/\sqrt{2}\,, \qquad (10)$$

which corresponds to the ground state of a particle in the absence of an electric field [13],[14].

Fig.1 shows the results of the solution of equations (4), (5) for some values of parameter κ, responsible for the intensity of the charge interaction with lattice oscillations at the electric field intensity $E=\mathcal{E}ea\tau/\hbar=0.1$, $\widetilde{\omega}=\omega\tau=0.01$, $\eta=1.276$. Here the values of parameters ω and η are the same as in work [12], and $\tau=10^{-14}$sec. In dimensional units these parameter values correspond

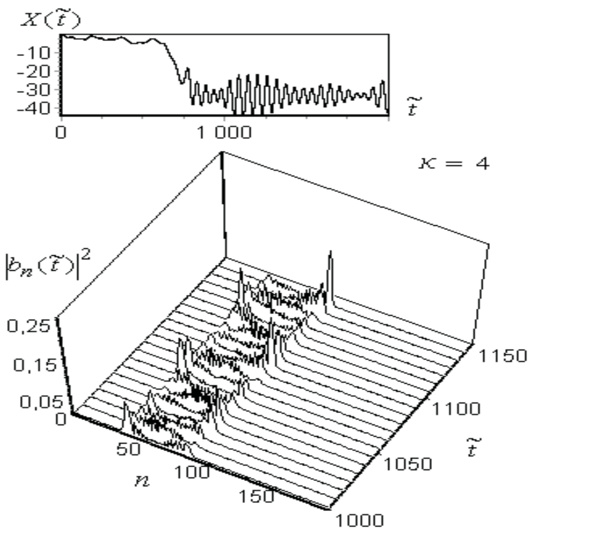

Fig. 2. Transition of a soliton into a breather for $\kappa = 4$. (Fig.1 d) at large times.)

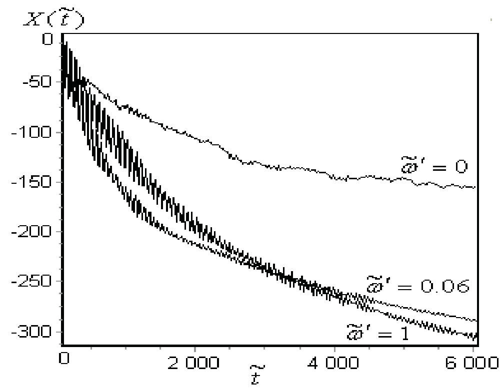

Fig. 3. Function $X(\widetilde{t})$ for various values of $\widetilde{\omega}\,'$.

to $\mathcal{E} = 1.94 \cdot 10^5 V/cm$, $\omega = \sqrt{k/M} = 10^{12} sec^{-1}$, $\nu = 0.084eV$. The parameter of electron-phonon strength $\kappa = 4$, which in dimensional units corresponds to $\alpha' = 0.13eV/\AA$ is the same as in [12]. This value is close to that used by other authors (in [18] α' was found to be $\alpha' \approx 0.23eV/\AA$).

It is seen from Fig.1 a) that in the presence of an electric field, a soliton executes periodical motions, coming back to the point where the soliton center mass initially occurred. This oscillatory motion corresponds to Bloch oscillations with a period of $T = 2\pi/\omega_B$. The total amplitude of the oscillations L is close to that determined from the solution of linear problem (6) and is written as: $\Delta W a/E$, where $\Delta W = 4\eta$ stands for the width of the conductivity band equal to $\Delta W \tau/\hbar$ in dimension form. For the parameter values presented above $L \approx 51a$ (with the soliton characteristic size $\approx 10a$).

Fig.1 b)-d) shows evolution of the dynamical behavior of a soliton at the initial stages of the motion as parameter κ increases. After a lapse of time Bloch oscillations restore (restored Bloch oscillations are not given in Fig.1 b)-d)).

In the case of strong electric fields presented in Fig.1, a soliton executing Bloch oscillations with time turns to a breather oscillating at Bloch frequency (Fig.2). At rather large values of κ, a breather can arise from the initial soliton state immediately, i.e. by-passing the phase of Bloch oscillations as a whole.

Without going into details of nonstationary regimes of the particle motion in the cases under consideration we will restrict ourselves to mere qualitative description of the picture. It has been observed that the case of a deformable chain ($\alpha' \neq 0$) differs qualitatively from the limiting case of a rigid chain ($\alpha' = 0$) in that at finite α' the quantity $X(t)$ given by (7) grows infinitely at $t \to \infty$ (Fig.3). This result could have been guessed from the already mentioned analogy between the influence of a periodic external electric field on a particle and oscillations of phonons. Quite nontrivial is the finding that under this influence, in the case of a strong particle-phonons interaction, i.e. when a soliton is formed, Bloch oscillations of the particle persist in the electric field as oscillations of a soliton as a whole or a breather, depending on the system parameters.

In conclusion it may be said that this picture of the charge motion in a deformable molecular chain in a constant electric field at zero temperature $T = 0$ seems to be rather general: a positive charge introduced in the chain will move along the field executing Bloch oscillations. At finite temperatures a soliton or breather state will break thus leading to failure of Bloch oscillations. In this case motion of the charge over the chain will be infinite along the lines of the field and have an ordinary band character.

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